

Perfluorotriethylamine
359-70-6 | DTXSID40189464

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 708

Global applicability domain: Outside

Local applicability domain index: 1.90e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

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1,1'-Isopropylidenebis(4-(1,1,2,2-tetrafluoroethoxy)benzene)

Measured: 22400
Predicted: 356

Image not found

1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 2.51
Predicted: 2.40

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2,4-Dichlorobenzotrifluoride

Measured: 2340
Predicted: 108

Image not found

1,2-Dichloro-4-(trifluoromethyl)benzene

Measured: 1510
Predicted: 321

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2,2,4,6,6-Pentamethylheptane

Measured: 871
Predicted: 963